SECOST: sequence-conformation-structure database for amino acid residues in proteins

EXHIBIT F

Releas 3.0

Clean-up records with "artifact" data: ☑

Resolution of the PDB files (Å): 0.0 to 2.5

Crystallographic R-factor: 0.0 to 0.25

Fractional area for the current residue: 0.0 to

Configuration of the peptide group: ◉ any ○ TRANS ○ CIS

Pattern for Amino Acid Sequence:

i-4	*i-3*	*i-2*	*i-1*	*i (current)*	*i+1*	*i+2*	*i+3*
any	any	any	any	any	any	any	any
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
MET	MET	MET	MET	MET	MET	MET	MET
PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
SER	SER	SER	SER	SER	SER	SER	SER
THR	THR	THR	THR	THR	THR	THR	THR
TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP
TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
polar	polar	polar	polar	polar	polar	polar	polar
nonpolar	nonpolar	nonpolar	nonpolar	nonpolar	nonpolar	nonpolar	nonpol
charged+	charged+	charged+	charged+	charged+	charged+	charged+	charge
charged-	charged-	charged-	charged-	charged-	charged-	charged-	charge
small	small	small	small	small	small	small	small
aromatic	aromatic	aromatic	aromatic	aromatic	aromatic	aromatic	aromati

Polar: RNDCEQHKSTW **Non-polar:** ACGILKMFWY **Charged+:** RHK

Charged-: DE **Small:** ANDCGPST **Aromatic:** HFWY

Submit Reset **Help**

Pattern for Secondary Structur :

i-4	*i-3*	*i-2*	*i-1*	*i (current)*	*i+1*	*i+2*	*i+3*	*i+4*
any	any	any	any	any	any	any	any	any
-	-	-	-	-	-	-	-	-
p	p	p	p	p	p	p	p	p
P	P	P	P	P	P	P	P	P
b	b	b	b	b	b	b	b	b
B	B	B	B	B	B	B	B	B
e	e	e	e	e	e	e	e	e
E	E	E	E	E	E	E	E	E
g	g	g	g	g	g	g	g	g
G	G	G	G	G	G	G	G	G
h	h	h	h	h	h	h	h	h
H	H	H	H	H	H	H	H	H
i	i	i	i	i	i	i	i	i
I	I	I	I	I	I	I	I	I
t	t	t	t	t	t	t	t	t
T	T	T	T	T	T	T	T	T

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Pattern for Conformational Sequence:

i-4	*i-3*	*i-2*	*i-1*	*i (current)*	*i+1*	*i+2*	*i+3*	*i+4*
any	any	any	any	any	any	any	any	any
B	B	B	B	B	B	B	B	B
R	R	R	R	R	R	R	R	R
P	P	P	P	P	P	P	P	P
C	C	C	C	C	C	C	C	C
L	L	L	L	L	L	L	L	L
G	G	G	G	G	G	G	G	G
I	I	I	I	I	I	I	I	I
D	D	D	D	D	D	D	D	D
@	@	@	@	@	@	@	@	@

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Fields in the output file:

Protein:

☑ ID of the PDB file; ☐ Resolution; ☐ R-factor

Current Residue:

☑ Chain/Name & sequential number of the residue; ☐ Code of the next residue
☑ Phi, ☑ Psi, ☐ Chi1, ☐ Chi2, ☐ Chi3, ☐ Chi4, ☐ Omega, ☐ Zeta
☐ Fractional area; ☐ Energy by residue

☐ Number of residues in the 8 Å sphere
☐ One-letter code for secondary structure containing the residue
☐ Conformational cluster, its ☐ Prior and ☐ Posterior Probabilities
☐ Pattern for Amino Acid Sequence
☐ Pattern for Secondary Structure
☐ Pattern for Conformational Sequence
☑ Line number

Delaunay simplices:

Types: ☐ 1-1-1-1, ☐ 2-1-1, ☐ 2-2, ☐ 3-1, ☐ 4

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In case of any publication, the following article should be cited: Shats, O., Vaisman, I., Shats, A., and Sherman, S. **SECOST: Sequence-Conformation-Structure Database for Amino Acid Residues in Proteins**, *Bioinformatics,* Vol.**15** no. 6 1999, pp. 525-526.

Send your comments to ***ssherm@unmc.edu***

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